# P-04-51

# Oskarshamn site investigation

# Hydrochemical logging in KSH03A

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March 2004

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*Keywords:* Core drilled borehole, Groundwater, Water sampling, Chemical analyses.

# Abstract

Hydrochemical logging or so called tube sampling has been performed in the core drilled borehole KSH03A. The method is a fast and simple sampling technique to obtain information about the chemical composition of the water column along an open borehole. The equipment consists of an approximately 1,000 metres long polyamide tube divided into units of 50 metres.

The water content in each tube unit constituted one sample. Every other sample, with start from the upper most unit, was analysed according to SKB chemistry class 3 (excluding isotope options). Samples for isotope determination were collected and stored in a freezer at the time of sampling; $\delta^{18}O$, deuterium, $^{87}Sr$ and $\delta^{34}S$ from odd tube units and tritium, $\delta^{37}Cl$ and carbon isotopes from even tube units. Samples for determination of tritium, $\delta^{37}Cl$, $\delta^{18}O$ and deuterium were sent for analysis approximately three months after the performance of the hydrochemical logging in KSH03A. Results from the isotope determinations will be presented in a separate report.

The content of flushing water remaining in the borehole after drilling reached a peak in the middle part of the borehole where it was about 20%. The lowest value of remaining flushing water was found in the uppermost sections and in the deepest section where it was approximately 5%. The relative charge balance error did exceed the acceptable limit of ± 5% in the first two sections analysed counted from the ground level.

# Sammanfattning

Hydrokemisk loggning, eller så kallad slangprovtagning, har utförts i det kärnborrade borrhålet KSH03A. Metoden är snabb och enkel att använda för att erhålla information om den kemiska sammansättningen hos grundvattnet längs ett öppet borrhål. Utrustningen består av en cirka 1 000 meter lång polyamidslang uppdelad i enheter om vardera 50 meter.

Innehållet i en slangenhet utgör ett prov.

Varannan slangenhet, med start från den översta, analyserades enligt SKB kemiklass 3 (exklusive tillval). Prover för bestämning av isotoptillvalen togs ut vid provtagningstillfället och sparades i frys; $\delta^{18}$O, deuterium, $^{87}$Sr och $\delta^{34}$S ur udda enheter samt tritium, $\delta^{37}$Cl och kolisotoper ur jämna enheter. Prover för bestämning av isotoperna tritium, $\delta^{37}$Cl, $\delta^{18}$O och deuterium sändes till laboratorier för analys ungefär tre månader efter provtagningen i KSH03A. Resultaten av utförda isotopbestämningar kommer att presenteras i en separat P-rapport.

Halten kvarvarande spolvatten efter borrning av borrhålet var som högst i de mellersta delarna (cirka 20 %) och som lägst närmast markytan och i de djupaste delarna (omkring 5 %). Det relativa felet i jonbalansen översteg den acceptabla nivån av ± 5 % i de två översta analyserade sektionerna.

# Contents

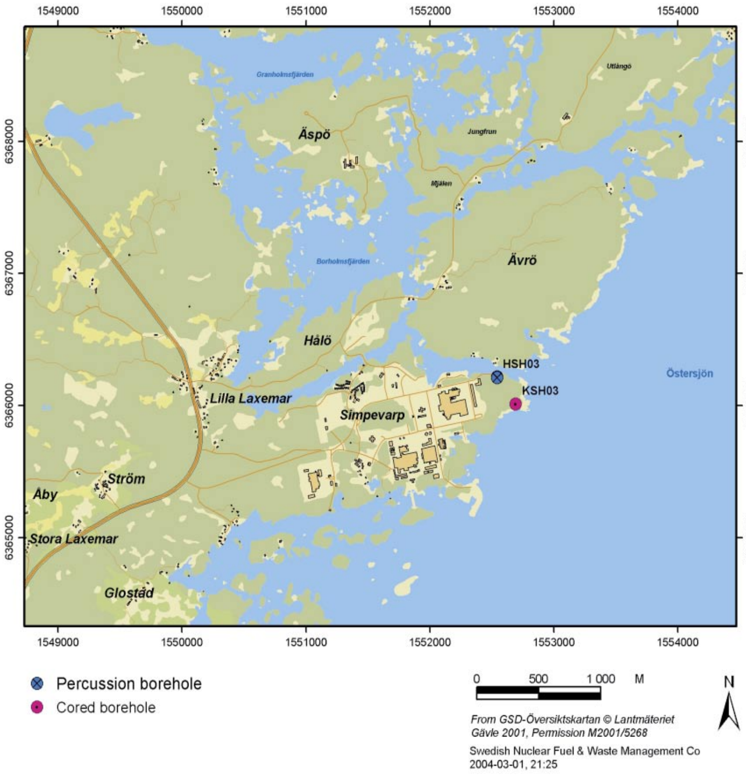
# 1 Introduction

The following document reports performance of and results from the activity "Hydrochemical logging in KSH03A", performed within the site investigation at Oskarshamn /1/. In Table 1-1 controlling dokuments for performing this activity are listed. Both activity plan and method description are SKB's internal controlling documents. The data is reported to SICADA in field note no Simpevarp 228.

**Table 1-1. Controlling documents for the performance of the activity.**

| **Activity plan** | **Number** | **Version** |
|---|---|---|
| *Hydrokemisk loggning i KSH03* | AP PS 400-03-059 | 1.0 |
| **Method description** | **Number** | **Version** |
| *Metodbeskrivning för hydrokemisk loggning* | SKB MD 422.001 | 1.0 |

Borehole KSH03A is a 1,000.77 metre long telescopic borehole drilled at the site investigation in the Oskarshamn area, Simpevarp The borehole has an inclination of about 59° at the top. The inclination decreases towards the bottom of the borehole where it is about 46°. The percussion borehole HSH03 served as source of flushing water for the core drilling of KSH03A. The location of KSH03A and HSH03 is shown in Figure 1-1.



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2004-03-01, 21:25

*__Figure 1-1.__ Location of the core borehole KSH03A and the supply well of flushing water HSH03 at the site investigation in the Oskarshamn area.*

# 2 Objective and scope

Hydrochemical logging was performed in order to obtain an overview of the chemical composition of the water along the open borehole KSH03A. The technique used for sampling is fast and simple even at great depth.

The analysis program was carried out according to SKB chemistry class 3 without options. Samples for analyses of isotopes were collected but not sent for analysis at the sampling occation. Samples for determination of the isotopes tritium, $\delta^{37}$Cl, deuterium and $\delta^{18}$O were stored in freezer until they were sent for analysis in the beginning of May, i.e. about three months after the hydrochemical logging. The results from these determinations will be presented in a separate report. The other collected isotope samples ($^{87}$Sr, $\delta^{34}$S and carbon isotopes) are still stored in a freezer at SKB Oskarshamn.

# 3 Sampling equipment

For the hydrochemichal logging an approximately 1000 metre long polyamide tube, divided into units of 50 metres, was used. The equipment is described in the method description SKB MD 422.001.

A schematic picture of the equipment used for the hydrochemichal logging is shown in Figure 3-1. The tube units are connected with couplings. The length of each tube unit is given in Table 3-1. The external and internal diameters of the tube units are 10 and 8 mm respectively. The water content in each tube unit constitutes one sample and the volume of each sample is approximately two and a half litres. At the lower end of the tube array, a weight is added to keep it stretched in the borehole and to prevent fastening. The first tube lowered down the borehole has a non return valve at the bottom to prevent water outflow while lifting the tube units. At both ends of each tube unit there is a manual shut off valve.

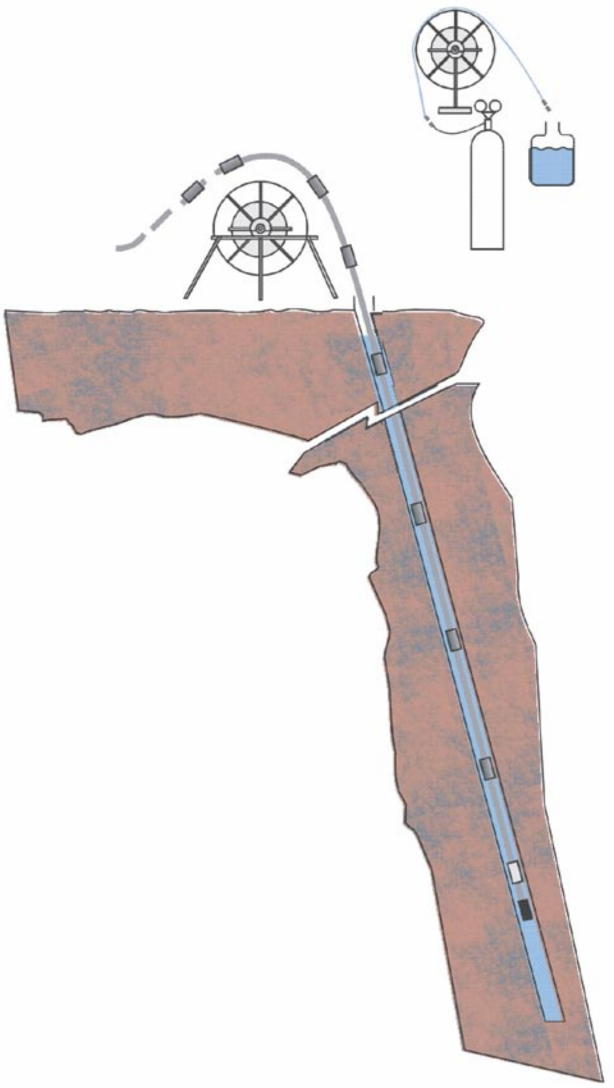

***Figure 3-1.*** *Equipment for hydrochemical logging in boreholes. At the lower end of the tube array there is a nonreturn valve and a weight connected. Each tube unit is 50 metres long.*

**Table 3-1. Length of tube units used at the hydrochemical logging in KSH03A.**

| Unit | Length (m) |
|---|---|
| 1 | 49.71 |
| 2 | 50.08 |
| 3 | 49.77 |
| 4 | 49.28 |
| 5 | 49.97 |
| 6 | 50.01 |
| 7 | 49.85 |
| 8 | 49.87 |
| 9 | 49.57 |
| 10 | 49.72 |
| 11 | 49.67 |
| 12 | 50.25 |
| 13 | 50.62 |
| 14 | 49.70 |
| 15 | 49.22 |
| 16 | 49.20 |
| 17 | 49.30 |
| 18 | 49.63 |
| 19 | 49.62 |
| 20 | 49.87 |
| **Sum** | 994.91 |
| **Couplings** | 2.812 |
| **Weight** | 0.817 |
| **Total tube length** | **998.539** |

# 4 Performance

## 4.1 Hydrochemical logging

The hydrochemichal logging in KSH03A was performed January 27, 2004.

Before the hydrochemical logging the ground water level was measured to 4.82 metres from the top of the casing. The first tube unit was lowered at 09:18. The tubes were lowered down the borehole at a rate of about five metres/minute. The equipment was lowered to a depth of 990 metre, i.e. the length of the borehole subtracted with 11 metres, to avoid suspending drilling debris sedimented at the bottom of the borehole and decrease the risk of fastening. The lifting of the tubes started at 13:32 and at 14:57 the last tube was lifted up. The tube unit at the top of the tube array was lowered to 40 metres of its length. This, and the fact that the groundwater level was at 4.82 metres below the top of the casing at the start of the hydrochemical logging, resulted in a not completely filled tube unit. The tube units were emptied using pressurized nitrogen gas and the water samples were portioned into sample bottles. Each tube unit represents one sample.

## 4.2 Sample treatment and chemical analyses

An overview of sample treatment and analysis routine is given in Appendix 1. The routines are applicable independent of sampling object or sampling method.

An overview showing the samples obtained at the logging occasion is given in Table 4-1. Sample portions intended for isotope analyses were collected but not sent for analyses at the time of the hydrochemical logging. Collected samples for tritium, $\delta^{37}$Cl, deuterium and $\delta^{18}$O were stored in freezer until they were sent to be analysed about three months after sampling occasion. The remaining samples collected for isotope determinations are still stored in freezer at SKB. The data from the hydrochemical logging are stored in the database SICADA in field note no Simpevarp 228. The SKB sample numbers are 7086–7105.

**Table 4-1. Overview of samples collected at the hydrochemical logging in KSH03A. Filled cells represents collected samples. Blue filling represents samples sent for analyses, light yellow filling represents samples collected and stored in freezer and purple dashed cells represents archive samples also stored in a freezer.**

| Sample information | | | Collected sample portions | | | | | | | | | Archive | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Tube unit | Length (m) | SKB no | Cond, pH, alk | Major comp | An-ions | Uranine | δ 2H/ δ18O | δ34S | 87Sr | 3H/ δ37Cl | Carbon isotopes | Filtered 250 mL | Unfiltered 250 mL |
| 1 | 0<br>40 | 7086 | 🟦 | 🟦 Relative charge balance error | 🟦 | 🟦 | 🟨 ж | 🟨 ω | 🟨 ж | | | | |
| 2 | 90 | 7087 | | | | | | | | 🟨 | 🟨 | | |
| 3 | 140 | 7088 | 🟦 | 🟦 Relative charge balance error | 🟦 | 🟦 | 🟨 | 🟨 | 🟨 | | | | |
| 4 | 190 | 7089 | | | | | | | | 🟨 | 🟨 | 🟪 | 🟪 |
| 5 | 240 | 7090 | 🟦 | 🟦 | 🟦 | 🟦 | 🟨 | 🟨 | 🟨 | | | | |
| 6 | 290 | 7091 | | | | | | | | 🟨 | 🟨 | 🟪 | 🟪 |
| 7 | 340 | 7092 | 🟦 | 🟦 | 🟦 | 🟦 | 🟨 | 🟨 | 🟨 | | | | |
| 8 | 390 | 7093 | | | | | | | | 🟨 | 🟨 | 🟪 | 🟪 |
| 9 | 440 | 7094 | 🟦 | 🟦 | 🟦 | 🟦 | 🟨 | 🟨 | 🟨 | | | | |
| 10 | 490 | 7095 | | | | | | | | 🟨 | 🟨 | 🟪 | 🟪 |
| 11 | 540 | 7096 | 🟦 | 🟦 | 🟦 | 🟦 | 🟨 | 🟨 | 🟨 | | | | |
| 12 | 590 | 7097 | | | | | | | | 🟨 | 🟨 | 🟪 | 🟪 |
| 13 | 640 | 7098 | 🟦 | 🟦 | 🟦 | 🟦 | 🟨 | 🟨 | 🟨 | | | | |
| 14 | 690 | 7099 | | | | | | | | 🟨 | 🟨 | 🟪 | 🟪 |
| 15 | 740 | 7100 | 🟦 | 🟦 | 🟦 | 🟦 | 🟨 | 🟨 | 🟨 | | | | |
| 16 | 790 | 7101 | | | | | | | | 🟨 | 🟨 | 🟪 | 🟪 |
| 17 | 840 | 7102 | 🟦 | 🟦 | 🟦 | 🟦 | 🟨 | 🟨 | 🟨 | | | | |
| 18 | 890 | 7103 | | | | | | | | 🟨 | 🟨 | 🟪 | 🟪 |
| 19 | 940 | 7104 | 🟦 | 🟦 | 🟦 | 🟦 | 🟨 | 🟨 | 🟨 | | | | |
| 20 | 990 | 7105 | | | | | | | | 🟨 | 🟨 | 🟪 | 🟪 |

ж filled with sample water from tube unit two.
ω partly filled with sample water from tube unit two.

All tube units, except for the upper most unit, seemed by eye to be fully filled. Only small bubbles of gas could be observed in the tube units. Due to the lack of water in the first tube unit, see above, archive samples from the second tube unit could not be filled. Water intended for archive samples in the second unit were used to fill sample bottles for deuterium/$\delta^{18}O$, $^{87}Sr/^{86}Sr$ and $\delta^{34}S$ from the first section (0–40 m).

Samples for isotope option of SKB chemistry class 3 were collected, but not sent for analyse. The sample bottles intended for various isotope analyses are stored at SKB for possible analyses later.

## 4.3 Data handling

The following routines for quality control and data management are generally applied for hydrogeochemical analysis data, independent of sampling method or sampling object.

Several components are determined by more than one method and/or laboratory. Moreover, control analyses by an independent laboratory are performed as a standard procedure on each fifth or tenth collected sample.

All analytical results were stored in the SICADA database. The applied hierarchy path "Hydrochemistry/Hydrochemical investigation/Analyses/Water in the database" contains two types of tables, raw data tables and primary data tables (final data tables).

Data on basic water analyses are inserted into raw data tables for further evaluation. The evaluation results in a final reduced data set for each sample. These data sets are compiled in a primary data table named "water composition". The evaluation is based on:

- Comparison of the results from different laboratories and/or methods. The analyses are repeated if a large disparity is noted (generally more than 10%).
- Calculation of charge balance errors. Relative errors within ± 5% are considered acceptable (in surface waters ± 10%).

$$\text{Rel. Error (\%)} = 100 \times \frac{(\sum \text{cations(equivalents)} - \sum \text{anions(equivalents)})}{(\sum \text{cations(equivalents)} + \sum \text{anions(equivalents)})}$$

- General expert judgement of plausibility based on earlier results and experiences.

All results from special analyses of trace metals and isotopes are inserted directly into primary data tables. In those cases where the analyses are repeated or performed by more than one laboratory, a "best choice" notation will indicate those results which are considered most reliable.

An overview of the data management is given in Figure 4-1.

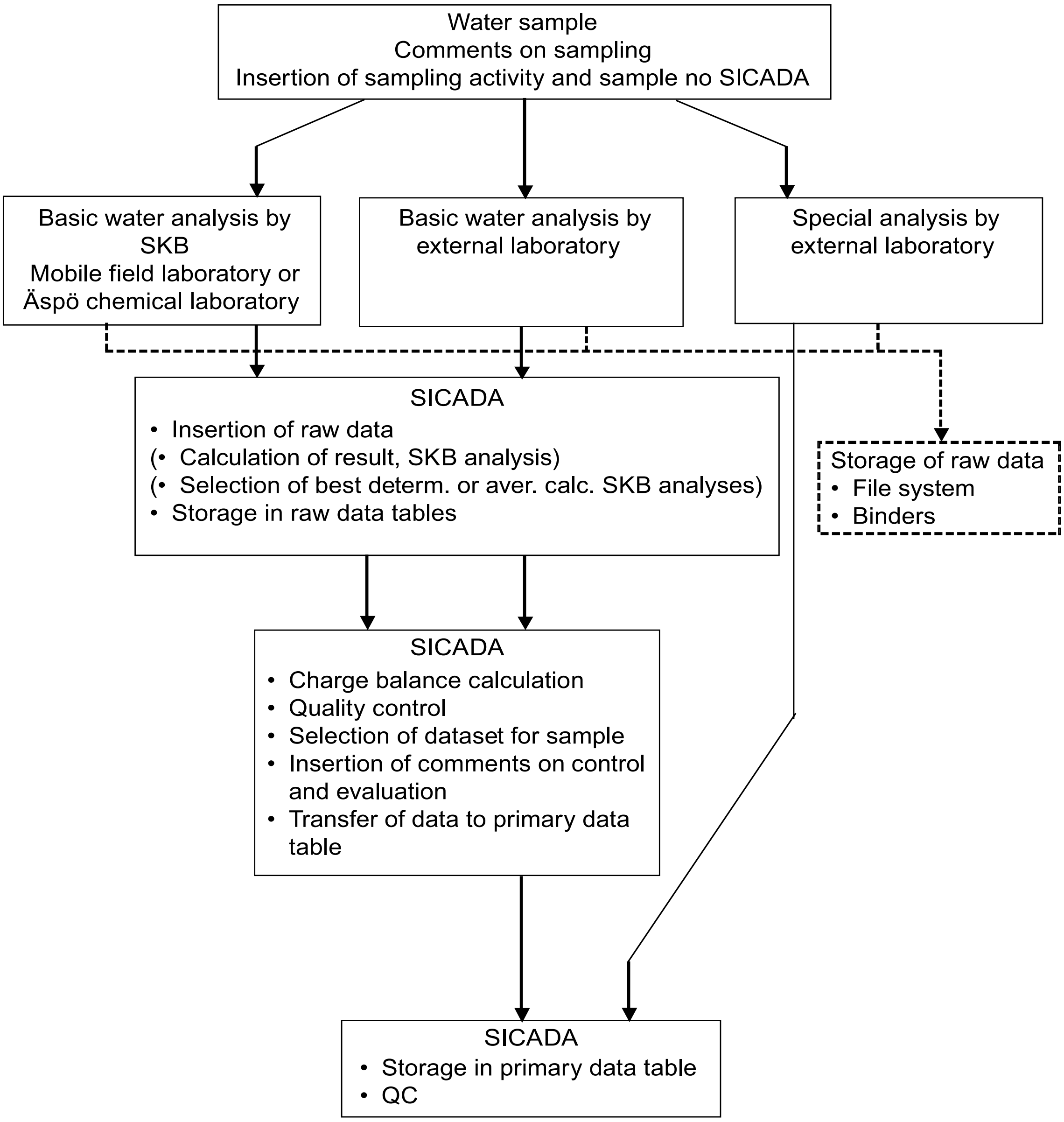

***Figure 4-1.** Overview of data management for hydrogeochemical data.*

## 4.4 Nonconformities

The activity was performed according without any deviations that may affect the quality of the data.

# 5 Results

## 5.1 Analysis results

Results from the different analysis are given in Appendix 2. Diagrams showing the flushing water content and the electric conductivity are presented in Figure 5-1 and 5-2 below. Results of analysis of pH, hydrogen carbonate, anions and major components are shown in diagrams 5-3 to 5-8 below. Results are plotted for the mid-length of each tube unit, for example the first tube is plotted at 20 metres.

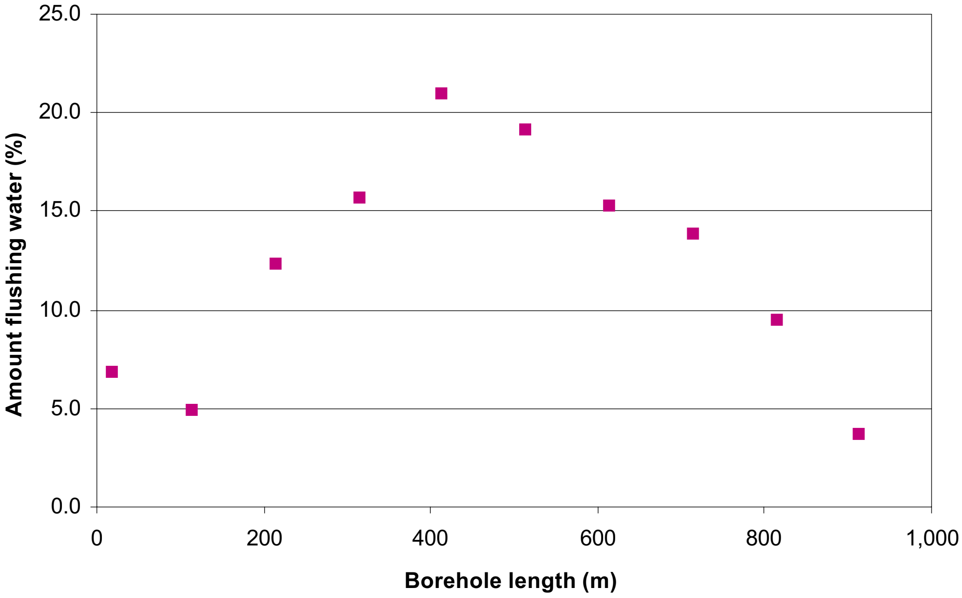

***Figure 5-1.*** *Amount of flushing water remaining at different lengths at the time of the hydrochemical logging in KSH03A.*

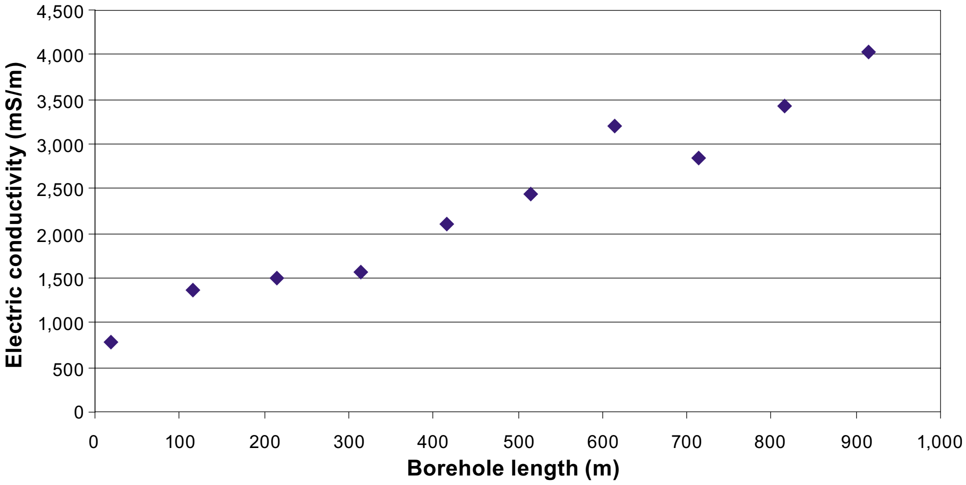

***Figure 5-2.*** *Electric conductivity values down the borehole KSH03A. Results from the hydrochemical logging, January 27, 2004.*

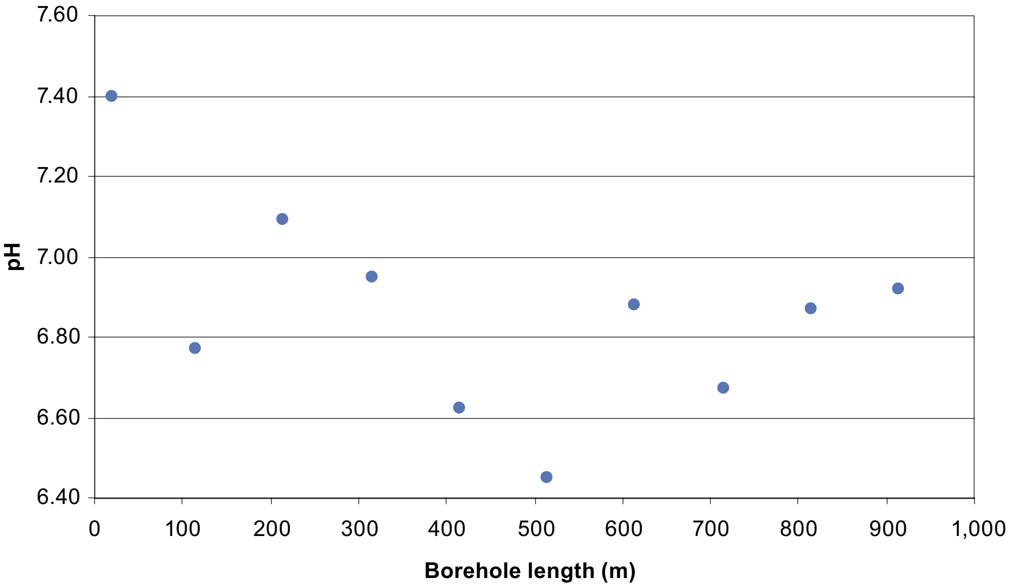

***Figure 5-3.*** *Results from pH measurements obtained from the hydrochemical logging in KSH03A.*

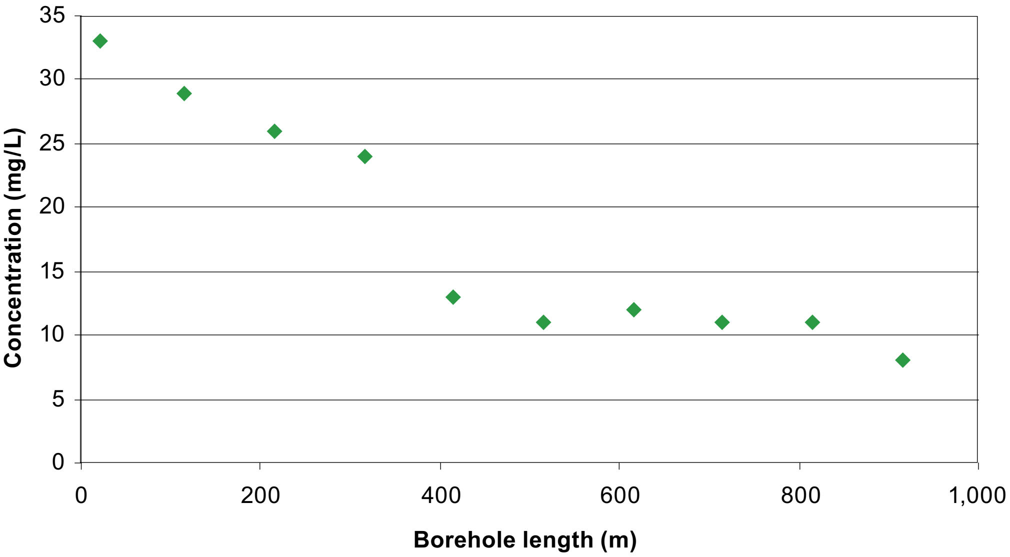

***Figure 5-4.*** *Results from hydrogen carbonate analysis of water samples taken at different depths in KSH03A January 27, 2004.*

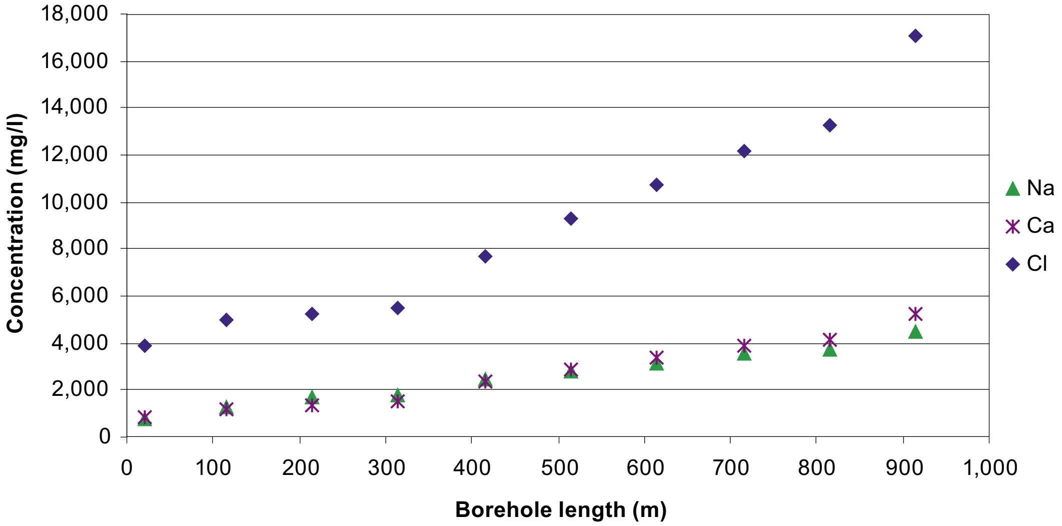

***Figure 5-5.*** *Analysis results from analysis of the components Na, Ca and Cl⁻ from water samples taken January 27, 2004.*

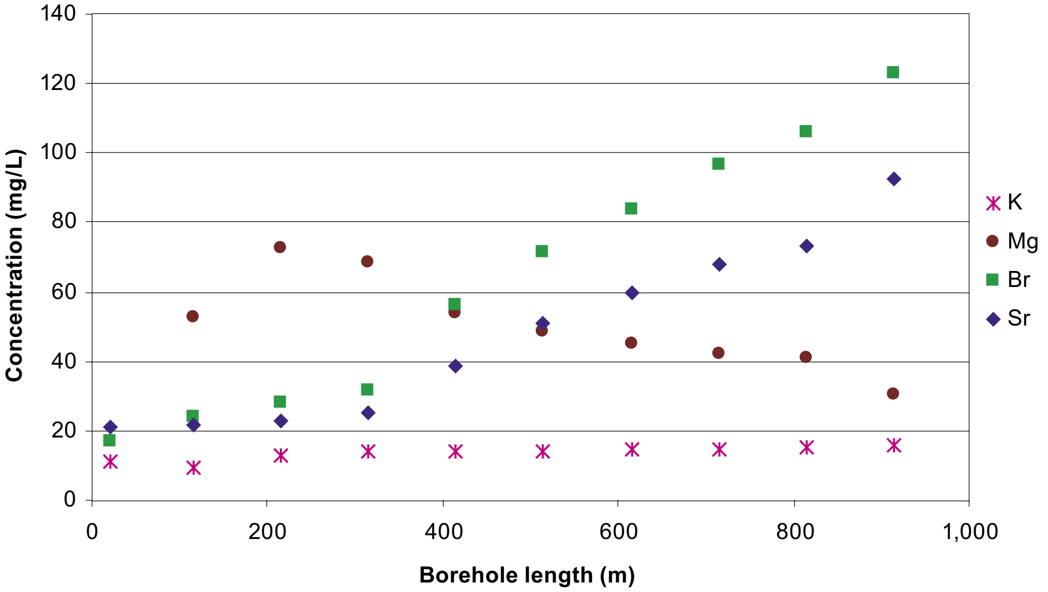

***Figure 5-6.*** *Results from analysis of K, Mg, Br and Sr. Data obtained from the hydrochemical logging in KSH03A.*

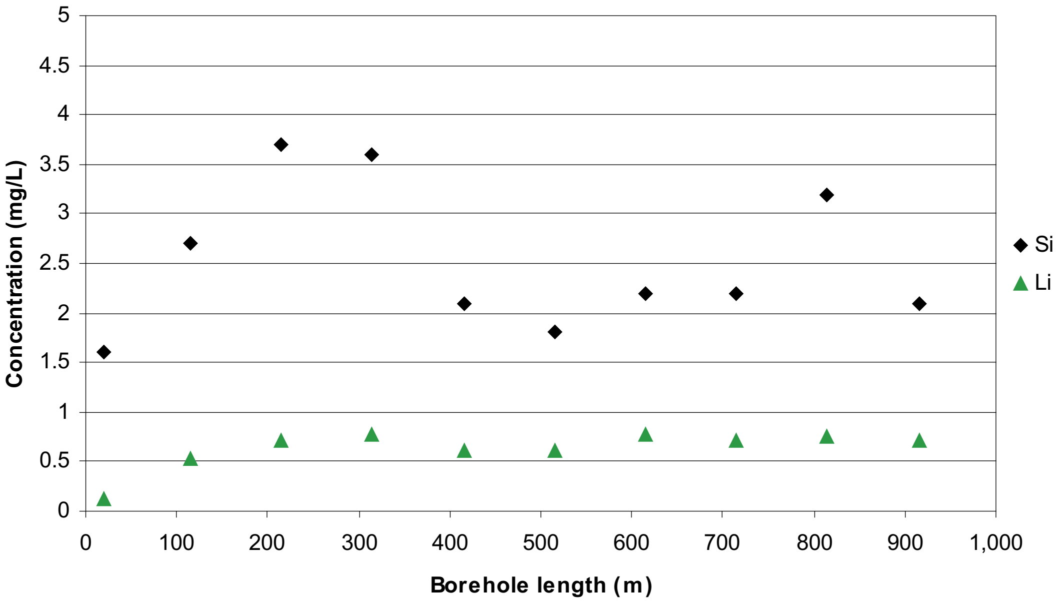

***Figure 5-7.** Concentrations of Si and Li obtained from samples taken January 27, 2004, at the hydrochemical logging in KSH03A.*

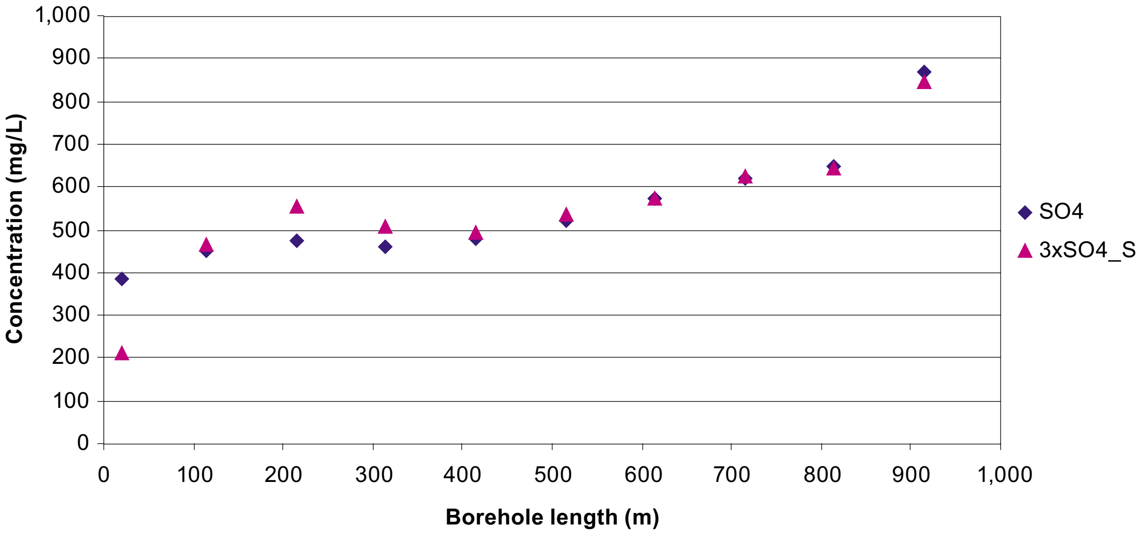

***Figure 5-8.** Sulphate (IC) compared to sulphate recalculated from total sulphur (ICP).*

Sulphate analysed by ion chromatography (IC) is compared to sulphate determined as total sulphur by ICP-AES in Figure 5-8. If sulphate is the only sulphur containing component, three times the total sulphur value should correspond to the sulfate concentration. As shown there is a satisfactory agreement except for the upper most section and the third section counted from the top of the borehole.

## 5.2 Quality of the analyses

The charge balance errors give an indication of the quality and uncertainty of the analyses of major components. The relative charge balance error are calculated for the selected sets of data, see Appendix 2. If the relative errors are within ±5% they are considered acceptable. The errors exceed 5% in 2 out of 10 cases, sample number 7086 and 7088.

Sample number 7098 were re-analysed at the consulted laboratory after doubtful results from the first analysis of the components Ca, Na and Sr. The re-analysis of the sample revealed that the lab had made a dilution error at the first analysis of the three components. This document reports the results from the second analysis of sample 7098.

# 6 Conclusions

At the hydrochemical logging in KSH03A the following chemical conditions was found:

- The amount of flushing water at the time of the hydrochemical logging had a maximum of 20% in the middle part of the borehole. The flushing water content is increasing down to this length and from 400 metres down to the bottom of the borehole the amount of remaining flushing water is decreasing. The lowest value was obtained from the sample collected at the deepest part sampled in the borehole i.e. section 940 to 990 metres.
- The charge balance error, giving an indication of the quality and uncertainty of the analyses, exceeded the acceptable level in two cases. The two samples, 7086 and 7088, with charge balance errors were from the first two sections analysed.
- The electric conductivity was increasing down the borehole.

# 7 Reference

/1/ **SKB, 2001.** Generellt genomförande program för platsundersökningar. SKB R-01-10, Svensk Kärnbränslehantering AB.

# Appendix 1

## Overview of sample treatment and analysis routines

**Table A1-1. Overview of general sample handling routines and analysis methods.**

| Component group | Component/ element | Sample container (material) | Volume (mL) | Filtering | Preparation/ Conservation* | Analysis method | Laboratory*** | Analysis within – or delivery time to lab. |
|---|---|---|---|---|---|---|---|---|
| Anions 1 | $HCO_3$<br>pH(lab)<br>cond (lab) | Plastic | 250 | Yes (not in the field) | No | Titration<br>Pot. meas,<br>Cond. meas | Mobile field lab<br>Alcontrol<br>Äspö's chemistry lab | The same day<br>– maximum 24 hours |
| Anions 2 | Cl, $SO_4$, $Br^-$, $F^-$, $I^-$ | Plastic | 100 | Yes (not in the field) | No | Titration ($Cl^-$)<br>IC ($Cl^-$, SO4, $Br^-$, $F^-$)<br>ISE ($F^-$) | Äspö's chemistry lab<br>Alcontrol | Not critical (month) |
|  | Br, I | Plastic | 100 | Yes (not in the field) | No | ICP MS | Paavo Ristola OY<br>SGAB Analytica, | Not critical (month) |
| Cations, Si and S according to SKB class 3 | Na, K, Ca, Mg, S(tot), Si(tot), Li, Sr | Plastic (at low conc acid washed bottles) | 100 | Yes (not in the field) | Yes (not in the field, 1 mL $HNO_3$) | ICP-AES<br>ICP-MS | SGAB Analytica,<br>SLU, Umeå | Not critical (month) |
| Cations, Si and S according to SKB class 4 and 5 | Na, K, Ca, Mg, S(tot), Si(tot), Fe, Mn, Li, Sr | Plastic (Acid washed) | 100 | Yes (immediately in the field) | Yes (1 mL $HNO_3$) | ICP-AES<br>ICP-MS | SGAB Analytica,<br>SLU, Umeå | Not critical (month) |
| Fe(II), Fe(tot) | Fe(II), Fe(tot) | Plastic (Acid washed) | 500 | Yes | Yes (5 mL HCl)) | Spectrophotometry<br>Ferrozine method | Mobile field lab | As soon as possible the same day |
| Hydrogen sulphide | HS– | Glass (Winkler) | About 120×2 | No | Ev 1 mL 1 M NaOH+ 1 mL 1M ZnAc | Spectrophotometry | Alcontrol<br>Äspö's chemistry lab | Immediately or if conserved, a few days |
| Nutrient salts | $NO_2$, $NO_3$+$NO_2$, $NH_4$, $PO_4$ | Plastic | 250 | No | No | Spectrophotometry | Äspö's chemistry lab<br>Alcontrol | Maximum 24 hours |

| Component group | Component/ element | Sample container (material) | Volume (mL) | Filtering | Preparation/ Conservation* | Analysis method | Laboratory*** | Analysis within – or delivery time to lab. |
|---|---|---|---|---|---|---|---|---|
| Environmental metals | Al, As, Ba, B, Cd, Co, Cr, Cu, Hg, Mo, Ni, P, Pb, V, Zn | Plastic | 100 | Yes | Yes (1 mL $HNO_3$) | ICP-AES<br>ICP-MS | SGAB Analytica, Alcontrol | Not critical (month) |
| Lantanoids, U, Th and so on. | Sc, Rb, Y, Zr, I, Sb, Cs, La, Hf, Tl, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, U, Th | Plastic | 100 | Yes | Yes (1 mL $HNO_3$) | ICP-AES<br>ICP-MS | SGAB Analytica,<br>Alcontrol | Not critical (month) |
| Dissolved organic Carbon, dissolved inorganic Carbon | DOC, DIC | Plastic | 250<br>25 | Yes | Frozen, transported in isolated bag | UV oxidation, IR Carbon analysator Shimadzu TOC5000 | Paavo Ristola OY Dept. of System ecology, SU | Short transportation time |
| Total organic Carbon | TOC | Plastic | 250<br>25 | No | Frozen, transported in isolated bag | UV oxidation, IR Carbon analysator Shimadzu TOC5000 | Paavo Ristola OY Dept. of System ecology, SU | Short transportation time |
| Environm01ental isotopes | $^{2}$H, $^{18}$O | Plastic | 100 | No | –<br>– | MS | IFE | Not critical (month) |
| Tritium, | $^{3}$H (enhanced.) | Plastic (dry bottle) | 500 | No | – | LSC | Univ Of Waterloo | Not critical (month) |
| Chlorine-37 | Chlorine-37 | Plastic | 100 | No | – | ICP MS | | |
| Carbon isotopes | $^{13}$C, $^{14}$C | Glass (brown) | 100×2 | No | – | (A)MS | Univ Of Waterloo | A few days |
| Sulphur isotopes | $^{34}$S | Plastic | 500–1,000 | Yes | – | Combustion, ICP MS | IFE | No limit |
| Strontium-isotopes | $^{87}$Sr/$^{86}$Sr | Plastic | 100 | Yes | – | TIMS | IFE | Days or Week |
| Uranium and Thorium isotopes | $^{234}$U, $^{235}$U, $^{238}$U, $^{232}$ Th, $^{230}$Th, | Plastic | 50 | Nej | – | Chemical separat. Alfa/ gamma spectrometry | IFE | No limit |
| Boron isotopes | $^{10}$B | Plastic | 100 | Yes | Yes (1 mL $HNO_3$) | ICP-MS | SGAB Analytica | No limit |
| Radon and Radium isotopes | $^{222}$Rn, $^{226}$Ra | Plastic | 500 | No | No | EDA, RD-200 | IFE | Immediate transport |

| Component group | Component/ element | Sample container (material) | Volume (mL) | Filtering | Preparation/ Conservation* | Analysis method | Laboratory*** | Analysis within – or delivery time to lab. |
|---|---|---|---|---|---|---|---|---|
| Dissolved gas (content and composition) | Ar, $N_2$, $CO_2$, $O_2$, $CH_4$, $H_2$, CO, $C_2H_2$, $C_2H_4$, $C_2H_6$, $C_3H_8$ | Cylinder of stainless steel | 200 | No | No | GC | Paavo Ristola OY | Immediate transport |
| Colloids | Filter series and fractionation (see below) | Polycarbonate filter | 0.45, 0.2 and 0.05 µm | – | $N_2$ atmosphere | ICP-AES<br>ICP-MS | SGAB Analytica | Immediate transport |
| Humic and fulvic acids | Fractionation | Fractions are collected in plastic bottles | 250 | – | $N_2$ atmosphere | UV oxidation, IR (DOC) | Paavo Ristola OY | Immediate transport |
| Archive samples with acid | – | Plast (washed in acid) | 100×2 ** | Yes | Yes (1 mL $HNO_3$) | – | – | Storage in freezer |
| Archive samples without acid | – | Plastic | 250×2 ** | Yes | No | – | – | Storage in freezer |
| Carbon isotopes in humic and fulvic acids | $^{13}C$, $^{14}C$ | DEAE cellulose (anion exchanger) | – | – | – | (A)MS | The Ångström laboratory, Uppsala | A few days |

* Suprapur acid is used for conservation of samples.

** Minimu□

*** Full name and address is given in Table A1-3.

**Abbreviations and definitions**

| | |
|---|---|
| IC | Ion chromatograph |
| ISE | Ion selective electrode |
| ICP-AES | Inductively Coupled Plasma Atomic Emission Spectrometry |
| ICP-MS | Inductively Coupled Plasma Mass Spectrometry |
| INAA | Instrumental Neutron Activation Analysis |
| MS | Mass Spectrometry |
| LSC | Liquid Scintillation Counting |
| (A)MS | (Accelerator) Mass Spectrometry |
| GC | Gas Chromatography |

## Table A1-2. Reporting limits and measurement uncertainties.

| Component | Method | Detection limit | Reporting limit or range | Unit | Measurement uncertainties [2] | ”Total” uncertaintiy [3] |
|---|---|---|---|---|---|---|
| $HCO_3$ | Alkalinity titration | 0.2 | 1 | mg/L | 4% | Time delay affects the results |
| $Cl^-$ | Mohr titration | 5 | 70 | mg/L | 5% | <10% |
| $Cl^-$ | IC | 0.2 | 0.5 | | 6% | 20% |
| $SO_4$ | IC | 0.2 | 0.5 | mg/L | 6% | 15% |
| $Br^-$ | IC | 0.2 | 0.7 | mg/L | 9% | 20% |
| $Br^-$ | ICP | – | 0.001–0.010[1] | | 15% | |
| $F^-$ | IC | 0.2 | 0.6 | mg/L | 10% | 20% |
| $F^-$ | Potentiometri | – | – | | – | – |
| $I^-$ | ICP | – | 0.001–0.010[1] | mg/L | 15% | 20% |
| Na | ICP | – | 0.1 | mg/L | 4% | 10% |
| K | ICP | – | 0.4 | mg/L | 6% | 15% |
| Ca | ICP | – | 0.1 | mg/L | 4% | 10% |
| Mg | ICP | – | 0.09 | mg/L | 4% | 10% |
| S(tot) | ICP | – | 0.16 | mg/L | 10% | 15% |
| Si(tot) | ICP | – | 0.03 | mg/L | 4% | 15% |
| Sr | ICP | – | 0.002 | mg/L | 4% | 15% |
| Li | ICP | – | 0.2–2[1] | µg/L | 10% | 20% |
| DOC | See tab 1 | – | 0.5 | mg/L | 8% | 30% |
| TOC | See tab 1 | – | 0.5 | mg/L | 10% | 30% |
| $\delta^{2}H$ | MS | – | 2 | ‰ dev SMOW[4] | 1.0‰ | – |
| $\delta^{18}O$ | MS | – | 0.1 | ‰ dev SMOW[4] | 2‰ | – |
| $^{3}H$ | LSC | – | 0.8 or 0.1 | TU[5] | 0.8 or 0.1 TU | – |
| $\delta^{37}Cl$ | ICP MS | – | 0.2‰ (20 mg/L) | ‰ SMOC[6] | – | – |
| $\delta^{13}C$ | A (MS) | – | >20 mg Carbon | ‰ PDB[7] | – | – |
| pmC ($^{14}C$) | A (MS) | – | >20 mg Carbon | pmC[8] | – | – |
| $\delta^{34}S$ | ICP MS | – | 0.2‰ | ‰ CDT[9] | 0.2‰ | – |
| $^{87}Sr/^{86}Sr$ | MS | – | – | No unit (ratio)[10] | 0.000020 | – |
| $^{10}B/^{11}B$ | ICP MS | – | – | No unit (ratio)[10] | 0.0020 | – |

[1] Reporting limits at salinity ≤ 0.4% (520 mS/m) and ≤ 3.5% (3810 mS/m) respectively.

[2] Measurement uncertainty reported by consulted laboratory.

[3] Estimated total uncertainty by experience (includes effects of sampling and sample handling).

[4] Per mill deviation[11] from SMOW (Standard Mean Oceanic Water).

[5] TU = Tritium Units, where one TU corresponds to a Tritium/hydrogen ratio of $10^{-18}$ (1 Bq/L Tritium = 8.45 TU).

[6] Per mill deviation[11] from SMOC (Standard Mean Oceanic Chloride).

[7] Per mill deviation[11] from PDB (the standard PeeDee Belemnite).

[8] The following relation is valid between pmC (percent modern carbon) and $^{14}C$ age:
$pmC = 100 \times e^{((1950-y-1.03t)/8274)}$.

[10] Isotope ration without unit.

[11] Isotopes are often reported as per mill deviation from standard. The deviation is calculated as:
$\delta^{y}I = 1{,}000 \times (K_{sample} - K_{standard})/K_{standard}$, where K = the isotope ratio and $^{y}I$ = $^{2}H$, $^{18}O$, $^{37}Cl$, $^{13}C$ or $^{34}S$ etc.

### Table A1-3. Consulted laboratories, full name and address.

Äspö waterchemical laboratory (SKB)
Mobile field laboratory, Forsmark (SKB)

Inainööritoimisto
Paavo Ristola Oy
Teollisuus-ja
Voimalaitoskemia
Rajantorpantie 8, C-talo
01600 Vantaa
FINLAND

Dept. of System ecology
Stockholm University
10691 Stockholm

Analytica AB
Aurorum 10
977 75 Luleå
(Nytorpsvägen 16
Box 511
183 25 Täby)

Environmental Isotope Laboratory
Dep. Of earth sciences
University of Waterloo
Waterloo, Ontario
N2L 3G1 CANADA

Institutt for energiteknik (IFE)
Insituttveien 18
P.O. Box 40
2027 Kjeller
NORGE

AnalyCen Nordic AB
Box 905
531 19 Lidköping

The Ångström laboratory
Box 534
SE-751 21 Uppsala

# Appendix 2

## Water composition, compilation of basic water analysis data

| Idcode | Secup m | Seclow m | Sample no | Charge Bal % | Na mg/L | K mg/L | Ca mg/L | Mg mg/L | $HCO_3^-$ mg/L | $Cl^-$ mg/L | $SO_4^{2-}$ mg/L | $SO_4$-S mg/L | $Br^-$ mg/L | $F^-$ mg/L | Si mg/L | Fe mg/L | Mn mg/L | Li mg/L | Sr mg/L | pH | Drill_water % | ElCond mS/m |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| KSH03A | 0 | 40 | 7,086 | –19.2 | 751 | 10.9 | 881 | 16.9 | 33 | 3,890 | 385 | 70.2 | 17.2 | <0.2 | 1.6 | 0.086 | 0.61 | 0.113 | 20.9 | 7.40 | 6.77 | 781 |
| KSH03A | 40 | 90 | 7,087 | | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| KSH03A | 90 | 140 | 7,088 | –11.6 | 1,300 | 9.4 | 1,200 | 52.9 | 29 | 4,970 | 451 | 155 | 24.3 | <0.2 | 2.7 | 0.091 | 0.71 | 0.532 | 21.9 | 6.77 | 4.91 | 1,370 |
| KSH03A | 140 | 190 | 7,089 | | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| KSH03A | 190 | 240 | 7,090 | –4.2 | 1,700 | 12.8 | 1,380 | 72.5 | 26 | 5,280 | 473 | 185 | 28.1 | <0.2 | 3.7 | 0.032 | 0.77 | 0.716 | 23.1 | 7.09 | 12.30 | 1,510 |
| KSH03A | 240 | 290 | 7,091 | | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| KSH03A | 290 | 340 | 7,092 | –2.5 | 1,790 | 13.8 | 1,510 | 68.5 | 24 | 5,490 | 460 | 169 | 31.5 | <0.2 | 3.6 | 2.290 | 0.73 | 0.764 | 25.3 | 6.95 | 15.70 | 1,560 |
| KSH03A | 340 | 390 | 7,093 | | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| KSH03A | 390 | 440 | 7,094 | –0.1 | 2,420 | 14.2 | 2,370 | 53.9 | 13 | 7,660 | 478 | 165 | 56.5 | <0.2 | 2.1 | 5.070 | 0.63 | 0.613 | 38.4 | 6.62 | 20.90 | 2,100 |
| KSH03A | 440 | 490 | 7,095 | | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| KSH03A | 490 | 540 | 7,096 | –0.7 | 2,800 | 14.2 | 2,910 | 48.9 | 11 | 9,270 | 523 | 178 | 71.3 | <0.2 | 1.8 | 4.900 | 0.58 | 0.618 | 51.1 | 6.45 | 19.10 | 2,430 |
| KSH03A | 540 | 590 | 7,097 | | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| KSH03A | 590 | 640 | 7,098 | –1.8 | 3,100 | 14.6 | 3,350 | 45.2 | 12 | 10,700 | 573 | 191 | 84.0 | <0.2 | 2.2 | 3.210 | 0.54 | 0.580 | 59.6 | 6.88 | 15.20 | 3,200 |
| KSH03A | 640 | 690 | 7,099 | | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| KSH03A | 690 | 740 | 7,100 | –1.6 | 3,520 | 14.5 | 3,850 | 42.3 | 11 | 12,200 | 621 | 208 | 96.9 | <0.2 | 2.2 | 1.970 | 0.52 | 0.707 | 67.9 | 6.67 | 13.8 | 2,850 |
| KSH03A | 740 | 790 | 7,101 | | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| KSH03A | 790 | 840 | 7,102 | –2.2 | 3,760 | 15.0 | 4,170 | 40.9 | 11 | 13,300 | 650 | 214 | 106 | <0.2 | 3.2 | 0.890 | 0.49 | 0.761 | 73.4 | 6.87 | 9.42 | 3,420 |
| KSH03A | 840 | 890 | 7,103 | | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| KSH03A | 890 | 940 | 7,104 | –4.6 | 4,490 | 15.9 | 5,240 | 30.4 | 8 | 17,100 | 870 | 281 | 123 | <0.2 | 2.1 | 0.766 | 0.41 | 0.716 | 92.3 | 6.92 | 3.68 | 4,040 |
| KSH03A | 940 | 990 | 7,105 | | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |

| Idcode | Secup m | Seclow m | Sample no | δ $^{2}$H dev SMOW | δ$^{18}$O dev SMOW | $^{3}$H TU | δ$^{37}$Cl dev SMOC | $^{10}$B/$^{11}$B no unit | $^{87}$Sr/$^{86}$Sr no unit | δ$^{34}$S dev CDT | δ$^{13}$C dev PDB | $^{14}$C pmC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| KSH03A | 0 | 40 | 7,086 | xxx | xxx | – | – | xxx | xxx | xxx | – | – |
| KSH03A | 40 | 90 | 7,087 | – | – | xxx | xxx | – | – | – | xxx | xxx |
| KSH03A | 90 | 140 | 7,088 | xxx | xxx | – | – | xxx | xxx | xxx | – | – |
| KSH03A | 140 | 190 | 7,089 | – | – | xxx | xxx | – | – | – | xxx | xxx |
| KSH03A | 190 | 240 | 7,090 | xxx | xxx | – | – | xxx | xxx | xxx | – | – |
| KSH03A | 240 | 290 | 7,091 | – | – | xxx | xxx | – | – | – | xxx | xxx |
| KSH03A | 290 | 340 | 7,092 | xxx | xxx | – | – | xxx | xxx | xxx | – | – |
| KSH03A | 340 | 390 | 7,093 | – | – | xxx | xxx | – | – | – | xxx | xxx |
| KSH03A | 390 | 440 | 7,094 | xxx | xxx | – | – | xxx | xxx | xxx | – | – |
| KSH03A | 440 | 490 | 7,095 | – | – | xxx | xxx | – | – | – | xxx | xxx |
| KSH03A | 490 | 540 | 7,096 | xxx | xxx | – | – | xxx | xxx | xxx | – | – |
| KSH03A | 540 | 590 | 7,097 | – | – | xxx | xxx | – | – | – | xxx | xxx |
| KSH03A | 590 | 640 | 7,098 | xxx | xxx | – | – | xxx | xxx | xxx | – | – |
| KSH03A | 640 | 690 | 7,099 | – | – | xxx | xxx | – | – | – | xxx | xxx |
| KSH03A | 690 | 740 | 7,100 | xxx | xxx | – | – | xxx | xxx | xxx | – | – |
| KSH03A | 740 | 790 | 7,101 | – | – | xxx | xxx | – | – | – | xxx | xxx |
| KSH03A | 790 | 840 | 7,102 | xxx | xxx | – | – | xxx | xxx | xxx | – | – |
| KSH03A | 840 | 890 | 7,103 | – | – | xxx | xxx | – | – | – | xxx | xxx |
| KSH03A | 890 | 940 | 7,104 | xxx | xxx | – | – | xxx | xxx | xxx | – | – |
| KSH03A | 940 | 990 | 7,105 | – | – | xxx | xxx | – | – | – | xxx | xxx |

– = Not analysed

A =Results will be reported later

x = No result due to sampling problems

xx = No result due to analytical problems

xxx = Sample stored in freezer

< = Result below detection limit

ChargeBal % = Relative charge balance error %

| IDCODE | Secup m | Seclow m | Sample no | Rel charge balance | Na mg/L | K mg/L | Ca mg/L | Mg mg/L | $HCO_3$ mg/L | Cl mg/L | $SO_4^{2-}$ mg/L | $SO_4$–S mg/L | Br mg/l | F mg/L | Si mg/L | Fe mg/L |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| KSH03A | 0 | 40 | 7,086 | –19.2 | 751 | 10.9 | 881 | 16.9 | 33 | 3,890 | 385 | 70.2 | 17.2 | <0.2 | 1.6 | 0.086 |
| KSH03A | 90 | 140 | 7,088 | –11.2 | 1,300 | 9.4 | 1,200 | 52.9 | 29 | 4,970 | 451 | 155 | 24.3 | <0.2 | 2.7 | 0.091 |
| KSH03A | 190 | 240 | 7,090 | –4.2 | 1,700 | 12.8 | 1,380 | 72.5 | 26 | 5,280 | 473 | 185 | 28.1 | <0.2 | 3.7 | 0.032 |
| KSH03A | 290 | 340 | 7,092 | –2.5 | 1,790 | 13.8 | 1,510 | 68.5 | 24 | 5,490 | 460 | 169 | 31.5 | <0.2 | 3.6 | 2.290 |
| KSH03A | 390 | 440 | 7,094 | –0.1 | 2,420 | 14.2 | 2,370 | 53.9 | 13 | 7,660 | 478 | 165 | 56.5 | <0.2 | 2.1 | 5.070 |
| KSH03A | 490 | 540 | 7,096 | –0.7 | 2,800 | 14.2 | 2,910 | 48.9 | 11 | 9,270 | 523 | 178 | 71.3 | <0.2 | 1.8 | 4.900 |
| KSH03A | 590 | 640 | 7,098 | –1.8 | 3,100 | 14.6 | 3,350 | 45.2 | 12 | 10,700 | 573 | 191 | 84.0 | <0.2 | 2.2 | 3.210 |
| KSH03A | 690 | 740 | 7,100 | –1.6 | 3,520 | 14.5 | 3,850 | 42.3 | 11 | 12,200 | 621 | 208 | 96.9 | <0.2 | 2.2 | 1.970 |
| KSH03A | 790 | 840 | 7,102 | –2.2 | 3,760 | 15.0 | 4,170 | 40.9 | 11 | 13,300 | 650 | 214 | 106 | <0.2 | 3.2 | 0.890 |
| KSH03A | 890 | 940 | 7,104 | –4.6 | 4,490 | 15.9 | 5,240 | 30.4 | 8 | 17,100 | 870 | 281 | 123 | <0.2 | 2.1 | 0.766 |

| IDCODE | Secup m | Seclow m | Sample no | Rel charge balance | Mn mg/L | Li mg/L | Sr mg/L | pH | ElCond mS/m | Flushing water % |
|---|---|---|---|---|---|---|---|---|---|---|
| KSH03A | 0 | 40 | 7,086 | –19.2 | 0,61 | 0,113 | 20,9 | 7,40 | 781 | 6,77 |
| KSH03A | 90 | 140 | 7,088 | –11.2 | 0,71 | 0,532 | 21,9 | 6,77 | 1370 | 4,91 |
| KSH03A | 190 | 240 | 7,090 | –4.2 | 0,77 | 0,716 | 23,1 | 7,09 | 1510 | 12,30 |
| KSH03A | 290 | 340 | 7,092 | –2.5 | 0,73 | 0,764 | 25,3 | 6,95 | 1560 | 15,70 |
| KSH03A | 390 | 440 | 7,094 | –0.1 | 0,63 | 0,613 | 38,4 | 6,62 | 2100 | 20,90 |
| KSH03A | 490 | 540 | 7,096 | –0.7 | 0,58 | 0,618 | 51,1 | 6,45 | 2430 | 19,10 |
| KSH03A | 590 | 640 | 7,098 | –1.8 | 0,54 | 0,580 | 59,6 | 6,88 | 3200 | 15,20 |
| KSH03A | 690 | 740 | 7,100 | –1.6 | 0,52 | 0,707 | 67,9 | 6,67 | 2850 | 13,8 |
| KSH03A | 790 | 840 | 7,102 | –2.2 | 0,49 | 0,761 | 73,4 | 6,87 | 3420 | 9,42 |
| KSH03A | 890 | 940 | 7,104 | –4.6 | 0,41 | 0,716 | 92,3 | 6,92 | 4040 | 3,68 |